Supersolid phases in the one dimensional extended soft core Bosonic Hubbard model

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We present results of Quantum Monte Carlo simulations for the soft core extended bosonic Hubbard model in one dimension exhibiting the presence of supersolid phases similar to those recently found in two dimensions. We find that in one and two dimensions, the insulator-supersolid transition has dynamic critical exponent $z = 2$ whereas the first order insulator-superfluid transition in two dimensions is replaced by a continuous transition with $z = 1$ in one dimension. We present evidence that this transition is in the Kosterlitz-Thouless universality class and discuss the mechanism behind this difference. The simultaneous presence of two types of quasi long range order results in two soliton-like dips in the excitation spectrum.

Experimental and theoretical work on supersolidity (SS), a thermodynamically stable phase in which diagonal (density) and off-diagonal (superfluid) order coexist [1], has seen an enormous resurgence over the past several years. In the case of solid Helium, the observation of an anomalous moment of inertia [2] has been vigorously re-investigated by several groups both experimentally [3] and theoretically [4]. In parallel, an entirely new arena for the investigation of supersolid phenomena has arisen in the context of cold atoms in optical lattices, whose description by the bosonic Hubbard Hamiltonian is well established [5]. It is known that this model does not exhibit supersolid phases due to the absence of longer range interactions. However, the recent realization [6] of Bose-Einstein condensate of ^{52}Cr atoms, which have an exceptionally large magnetic dipole moment and therefore long-range interactions, has opened wide the possibility of experimantal observation of SS phases on confined optical lattices [7].

Such strongly dipolar ultra-cold atoms, when placed on optical lattices, are governed by the *extended* Bosonic Hubbard Hamiltonian which has been shown, via extensive Quantum Monte Carlo (QMC) simulations, to exhibit SS phases in two dimensions. The model we consider is,

$$H = -t \sum_{<ij>} \left(a_i^\dagger a_j + a_j^\dagger a_i \right) + \frac{U}{2} \sum_i n_i(n_i - 1)$$
$$+V \sum_{<ij>} n_i n_j. \tag{1}$$

The hopping parameter, t, sets the energy scale, $n_i = a_i^\dagger a_i$ and $[a_i, a_j^\dagger] = \delta_{ij}$ are bosonic creation and destruction operators. The repulsive contact (near neighbor) interaction is U (V). Recently, it was shown [8] in $2d$ that the model described by Eq. (1) has a SS phase if U and V are such that when the charge density wave (CDW) phase is doped *above* half filling, the added bosons go on already occupied sites (roughly $U < 4V$). Doping
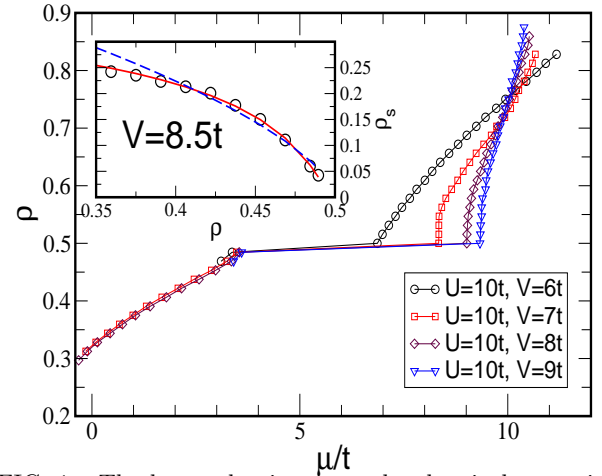

FIG. 1: The boson density, ρ, vs the chemical potential, μ, for $L = 64$, $\beta = 20$ with 200 time slices. Inset: ρ_s vs ρ as $\rho = 1/2$ is approached from below. See text near Eq. (6).

below half filling provokes phase separation and a first order transition to a SF phase. If multiple occupancy is suppressed, there is phase separation when the system is doped above half filling as in the hard core case[9]. This raises the possibility that an analogous phase exists for the one dimensional form of Eq. (1) in which case this would be the first example of a SS in a one dimensional system.

In this letter we re-examine the one dimensional soft core bosonic Hubbard model [11, 12], Eq. (1) under the same conditions. We conclude that a ground state SS phase does exist with similarities to, and important differences from, that in $2d$. Calculations of the excitation spectra and Landau critical velocity demonstrate that the SS phase is stable, and allow us to infer the dynamic critical exponents. We use the World Line algorithm in our QMC simulations.

We begin by demonstrating that for V sufficiently

large, the system has gapped, incompressible CDW insulating behavior at half-filling, $\rho = 1/2$. Figure 1 shows ρ vs μ for $U = 10t$ and $V = 6t$, $7t$, $8t$, $9t$ using the WL algorithm. The plateau at $\rho = 1/2$ clearly indicates a non-zero gap for all four cases. However, the behavior of the system depends on whether it is doped below or above $\rho = 1/2$, and on the value of V. Starting with the CDW and *removing* a particle creates a "defect" with three adjacent unoccupied sites which then splits into two mobile two-hole bound states (solitons) which destroy the long range CDW order in favor of quasi-long range order with $\rho_s \neq 0$. Consequently, all the curves coincide for $\rho < 1/2$ in Fig 1. In contradistinction, when the $2d$ CDW phase is doped below half filling, phase separation takes place leading to a first order phase transition. Upon *adding* a particle to the CDW for $V \leq 6t$, the extra particle goes to an unoccupied site since the cost of multiple occupancy exceeds that of near neighbors. Thus, a defect of three adjacent occupied sites is created which then splits into two mobile two-particle bound states (solitons) which are the particle-hole symmetric analogs of the $\rho < 1/2$ case. This particle-hole symmetry, seen for $V = 6t$ in Fig. 1, is of course approximate for finite U. On the other hand, upon adding a particle to the CDW when $V > 6t$, the cost of near neighbors exceeds that of multiple occupancy, and the extra particle goes to an already occupied site (which cannot happen in the hardcore case). This breakdown of particle-hole symmetry is seen for $V = 7t, 8t, 9t$ in Fig. 1. For $\rho > 1/2$ the curve first rises very sharply hinting at a diverging compressibility, $\kappa = \partial \rho / \partial \mu$ which is not the case for $\rho < 1/2$. We shall return to this point below.

In order to characterise the phases, we calculate the SF density, ρ_s [15], and the structure factor, $S(k)$,

$$\rho_s = \frac{\langle W^2 \rangle}{2t\beta L^{d-2}}, \qquad (2)$$

$$S(k) = \frac{1}{L^2} \sum_{x,x'} e^{ik(x-x')} \langle n(x)n(x') \rangle, \qquad (3)$$

where W is the winding number, L the length of the system, d the dimension and $\langle n(x)n(x') \rangle$ is the density-density correlation function. Figure 2(a) shows ρ_s versus ρ for $U = 10t$ and $V = 6t, 7t, 8t, 9t$ while 2(b) shows $S(k = \pi)$ for the same values. For $\rho < 0.5$, $S(\pi)$ is essentially zero, *i.e.* there is no CDW, while at the same time $\rho_s \neq 0$. This is a SF phase. This behavior is *qualitatively different* from that in two dimensions [8, 9] where the system undergoes phase separation and a first order transition. Such phase separation cannot happen in one dimension, and indeed Fig. 1 does not exhibit any negative compressibility regions [9]. Instead, solitonic excitations are produced [12].

For $\rho > 0.5$ and $V > 6t$, $S(\pi)$ takes non-zero values indicating simultaneous co-existence of SF and long range CDW order, in other words a SS in one dimension. That this SS does not undergo phase separation is again
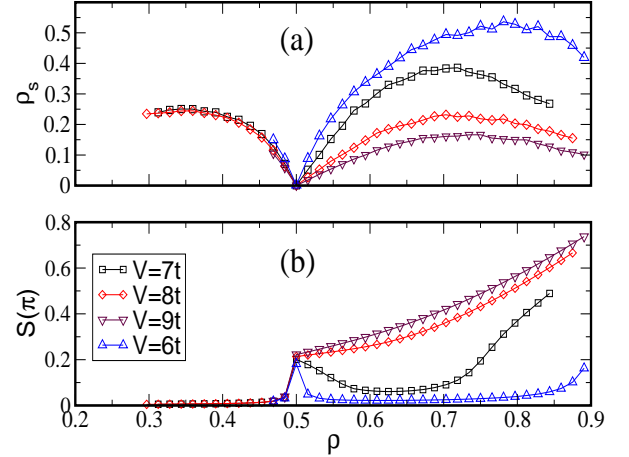

FIG. 2: (a) The superfluid density, ρ_s, and (b) the structure factor, $S(k)$, as functions of the number density ρ for four values of V. $L = 64$ sites, $\beta = 20$ and $U = 10t$.

clear from Fig. 1 where [9] the compressibility, κ is never negative. For $V = 7t$, finite size scaling shows that in the thermodynamic limit, ρ_s maintains a non-zero value whereas the behavior of $S(\pi)$ depends on ρ as $L \to \infty$. In other words, as this system is doped above half filling, it first enters a SS phase, then a SF phase and finally back into a SS. The phase diagram in two dimensions (Fig. 1 in Ref. [8]) does not exhibit such re-entrant behavior. On the other hand, for $V = 8t, 9t$, the system remains in the SS phase for all $\rho > 0.5$, at least up to the highest density we studied, $\rho = 1.1$, except at $\rho = 1$ where it is a gapped CDW insulator with alternating empty and doubly occupied sites.

The phase diagram for a fixed value of U in the $(\mu/t, t/V)$ plane is obtained by sweeping μ/t at constant t/V as shown in Fig. 1. This is shown in Fig. 3 for $U = 10t$. The phases and the nature of the transitions between them are explained in the caption. The details of the phase diagram above $\rho = 1$ have not been determined beyond establishing the natures of the phases just above the CDW-II and Mott-I as indicated in the figure. When CDW-II (Mott-I) is doped above or below $\rho = 1$, the system becomes supersolid (superfluid). We remark that in figure 3 ($U = 10t$) the CDW-II and Mott-I lobes have a very small contact region. This contact region increases as U is increased, *i.e.* the gap at the transition increases. On the other hand, if U is decreased, the two lobes separate and the direct transition between CDW-II and Mott-I is lost: a SF phase intervenes.

Having shown that supersolid phases exist, we turn now to the excitation spectrum, $\Omega(k)$ which, along with ρ_s, characterizes the superfluid phase. If $\Omega(k) \propto k$ for small k, excitations are phonons and the superfluid is said to be stable according to the Landau criterion: the
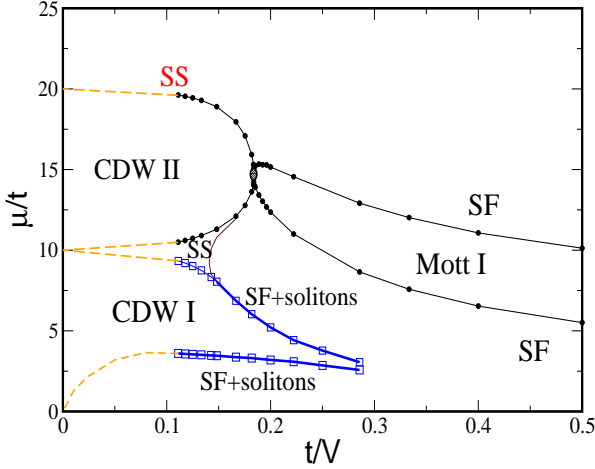
FIG. 3: The phase diagram for $U = 10t$. CDW-I is alternating empty and singly occupied sites, CDW-II is alternating empty and doubly occupied sites, Mott-I is the first Mott lobe with $\rho = 1$. Solid lines are second order transitions with $z = 2$; thick solid lines have $z = 1$ and appear to be in the KT universality class (see Eq. (6)); the CDW-II to Mott-I transition is first order. Dashed lines connect schematically the numerical results at the smallest t/V to the exact values at $t/V = 0$.

Landau critical velocity, v_c^L, is finite and is given by the slope of the line passing through the origin and tangent to the roton (or, for $d = 1$, the soliton) minimum. To obtain $\Omega(k)$, one can calculate, via QMC, the space and imaginary time separated density-density correlation function which then gives the dynamic correlation function. With the help of a numerical Laplace transform, for example using the Maximum Entropy method, $\Omega(k)$ can be obtained [16]. This procedure is demanding numerically. However, it was shown [16] that the rigorous Maxent procedure is not necessary since one obtains a good approximation (upper bound) for $\Omega(k)$ by using the f-sum rule leading to Feynman expression,

$$\Omega(k) = \frac{E_k}{LS(k)}. \tag{4}$$

where,

$$E_k = \frac{-t}{L}\left(\cos k - 1\right)\langle\Psi_0|\sum_{i=1}^{L}\left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i\right)|\Psi_0\rangle, \tag{5}$$

and $|\Psi_0\rangle$ is the ground state of the system.

Figure 4 shows $\Omega(k)$ vs k for several values of the density and interaction strength. The first three cases listed in the legend correspond to a fixed density $\rho = 15/32$, just below half filling in the SF phase. We note: (a) finite size effects are negligible, (b) $\Omega(k) \propto k$ as $k \to 0$, indicating phonon excitations and a stable SF, and (c) the soliton minimum is clearly visible at $k = 2.95$. As
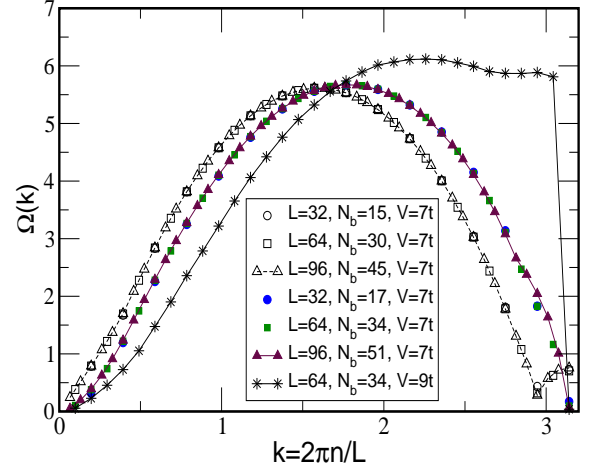

FIG. 4: The dispersion relation, $\Omega(k)$, vs the wave-vector, k, for several system sizes and boson numbers N_b. For all cases $U = 10t$.

$\rho \to 1/2$ from below, $\Omega(k)$ remains linear for small k but the soliton minimum moves towards $k = \pi$ and its energy approaches zero, pinching the k-axis, and signaling the CDW instability. Therefore, the Landau critical velocity, $v_c^L \to 0$ although the SF remains stable, with a high phonon velocity, all the way to the transition. The linearity of $\Omega(k)$ at the transition shows that the SF-CDW transition has a dynamic critical exponent $z = 1$.

The next three cases listed in the legend, Fig. 4, correspond to $\rho = 17/32$, just inside the SS phase. Again finite size effects are under control. In addition, we see that $\Omega(k)$ *softens* as $k \to 0$ and is no longer linear and that this effect increases with increasing V (the last case in Fig. 4). Fitting the form $\Omega(k) \propto k^z$ to the small k dispersion curves and sizes up to $L = 96$ for $\rho = 0.51$ gives $z \approx 1.9$. This suggests a dynamical critical exponent $z = 2$ for the CDW-SS transition. The same behavior is observed for $\Omega(k)$ as the $\rho = 1$ CDW-II phase (alternating doubly occupied and vacant sites) is approached from the SS phase above or below full filling, $\rho \to 1^\pm$. Therefore, the quantum phase transitions to the $\rho = 1/2$ CDW are different depending on whether they are approached from below ($\Omega(k \to 0) \propto k$ and soliton minimum pinching the k-axis) or from above ($\Omega(k)$ softens to a quadratic form). However, the transitions to the CDW-II phase, $\rho \to 1^\pm$, are in the same universality class with $z = 2$. We also have performed simulations in two dimensions and verified that the CDW-SS transition has $z = 2$.

Therefore, $\Omega(k)$ yields for the SF-CDW transition $z = 1$ while $z = 2$ for the SS-CDW transitions both at $\rho = 1/2$ and $\rho = 1$ (and presumably also for $\rho = 3/2$ etc). In addition, it was shown in Ref. [14, 17] that, when $V = 0$, ρ_s scales as $\rho_s \sim |\rho_c - \rho|^{z-1}$ with $z = 2$ where $\rho_c = 1, 2, ..$ is the density at which the MI phase is established. Our
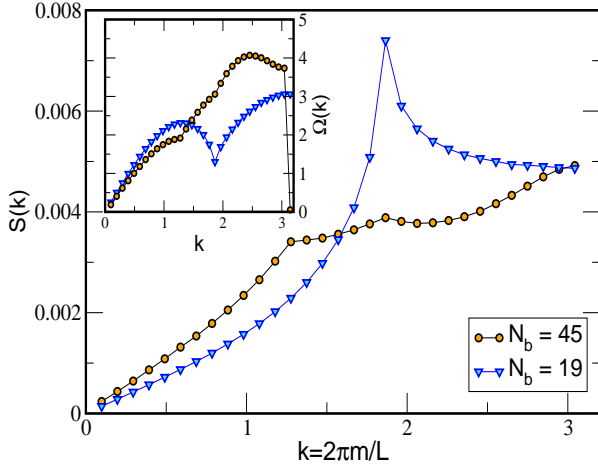
FIG. 5: Comparison of the structure factor, $S(k)$ for the same doping above and below half filling. $L = 64$, $\beta = 20$, $U = 10t$, $V = 8t$. Inset: The corresponding dispersion, $\Omega(k)$.

data show that for the SS-CDW $\rho_s \sim |\rho_c - \rho|^{0.95}$ again giving $z \approx 2$ assuming the same scaling law. On the other hand, for the SF-CDW transition $z = 1$ yielding $\rho_s \sim |\rho_c - \rho|^0$ ($\rho_c = 1/2$ here) which means that for this transition ρ_s does *not* vanish as a power law. In the absence of power law scaling, it is natural to attempt a Kosterlitz-Thouless (KT) scaling form,

$$\rho_s = A e^{-B/\sqrt{|\rho - \rho_c|}} \tag{6}$$

where A and B are nonuniversal constants. This is illustrated in the inset of Fig. 1 which shows ρ_s vs ρ for $L = 64, U = 10t, V = 8.5t$. The solid line is a two parameter fit with Eq. (6), the dashed line is a two parameter power law fit to the same points. The goodness of this fit suggest that this transition is in the KT universality class.

The dispersion curves in Fig. 4 show clearly that when the system is doped below $\rho = 1/2$, $\Omega(k)$ develops a soliton dip. Figure 5 shows the origin of this behavior. For $N_b = 19$, $\Omega(k)$ shows a pronounced minimum, while for $N_b = 45$ it shows two milder ones (inset Fig. 5). These excitation dips are caused by peaks in the structure factor which point to the presence of quasi long range order with the corresponding ordering vectors, $\mathbf{k}^*$. It is interesting to note that for $N_b = 45$ (and in general for $\rho > 1/2$) the structure factor $S(k)$ has two peaks (Fig. 5) indicating the simultaneous presence of two types of quasi long range order. It is clear from the figure that one of the peaks occurs at exactly the same $\mathbf{k}^*$ as the soliton peak for the same doping *below* half filling. This peak for $\rho > 1/2$ is caused by bosons occupying previously empty sites thus aquiring near neighbors even though the large value of V tries to suppress this. In other words, this is the vestige of the approximate particle-hole symmetry

present for $U = 10t$ and $V \le 6t$. The peak at the lower k comes from the quasi long range order produced when doubly occupied sites are produced. Recall that at full filling the ground state is a CDW with alternating doubly occupied and empty sites.

We now return to the behavior of the compressibility, $\kappa = \partial\rho/\partial\mu$, as $\rho \to 1/2^\pm$. It was argued in [14] for the SF-MI transition ($V = 0$, $\rho = 1$) that $\kappa \sim |\mu - \mu_c|^{\nu(d-z)}$, where μ_c is the chemical potential at the transition. For the $\rho \to 1/2^+$ transition, $(d = 1, z = 2)$, our preliminary results indicate $\kappa \sim |\mu - \mu_c|^{-0.6}$ which is consistent with $\nu = 1/2$ assuming the same scaling. For the $\rho \to 1/2^-$ transition $(d = 1, z = 1)$, this scaling yields $\kappa \sim |\mu - \mu_c|^0$ which means that, although $\kappa \to 0$ as $\rho \to 1/2^-$, it is not a power law.

In summary, we have presented QMC results showing that, contrary to previous results [11] where $U > 2V$, the extended one-dimensional soft core bosonic Hubbard model does have SS phases when doped above half filling when both U and V are large such that the system favors multiple rather than near nighbor occupancy. From the scaling of $\Omega(k)$, ρ_s and κ, we calculated the dynamic critical exponent, z, for all the transitions. We showed different universality classes due to the different behavior of $\Omega(k)$ depending on whether the CDW is approached from below or above half filling and we highlighted similarities and differences with the two dimensional case. Finally we note that $1d$ SS phases have been predicted for commensurate mixtures of two bosonic species, each near the hardcore limit, but where the interaction between the species is not too large[18].

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